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Five-site model for a motor protein walking on a bead-spring substrate NABINA PAUDYAL, MARAL ADELI KOUDEHI, JUTTA LUETTMER-STRATHMANN, University of Akron, Department of Physics — Motor proteins play an important role in many biological processes. For example, kinesin molecules are responsible for the transport of vesicles in nerve cells and their malfunction has been linked to neurodegenerative diseases. Motor proteins are also responsible for the unique mechanical properties of active matter. To study non-equilibrium aspects of motor-substrate systems, biological chain molecules interacting with motor proteins have been investigated in single-chain pulling experiments. Unfortunately, the complexity of motor proteins and their environment makes it difficult to model the detailed dynamics of molecular motors over long time scales. In this work, we develop a simple coarse-grained model for a motor protein on a bead-spring substrate under tension. In our model, different pair potentials describe interactions between substrate and motor, motor components and substrate components. The movement of motor proteins entails ATP hydrolysis, which is modeled in terms of mechano-chemical states that couple positional and chemical degrees of freedom. The goal of this work is to simulate cargo transport in confined geometries and to investigate the mechanical response of a single chain interacting with motor proteins.

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